Structure Determination of Pentacene Derivative by Synchrotron Powder Diffraction Data

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Organic thin-film transistors have attracted much attention for their potential application as alternatives to the traditional amorphous silicon-based TFTs. The pentacene derivative stands out as a promising material because of its ability to form ordered films and its reasonably high field-effect mobility and on/off ratio. Numerous efforts were attempted aiming at improving the electronic properties of pentacene-based devices. The crystal structure of the pentacene derivative thin film is the main theme to understand the physical properties and provide the base for theoretical calculation. We have solved the crystal structure of tetra chlorodiazapentacene (TCDAP) by synchrotron powder diffraction data. The compound is difficult to growth large enough crystal for single crystal diffraction study. From the powder diffraction data we found that TCDAP crystallize in monoclinic of space group P 2_1/n, a=17.0302(17), b=12.1166(11), c=4.0236(2)Å, beta=91.29(1), vol=930.06(9), Z=2. The unit cell is indexed by DICVOL. Structure determination from powder diffraction data was carried out using monte carlo simulation of DASH program. The final Rietveld refinement by GSAS program gave Rwp= 0.0675, Rp=0.0425, and X^2= 1.56. The powder structure of TCDAP fit well to its thin film diffraction pattern. Some other powder structures of pentacene derivatives are also under solving.